

a new insight in the complexity of *Transition-Metal (TM) oxides* in the regime of high density of matter.

(ii) At  $P > 45$  GPa a *high to low* spin crossover takes place of both iron species in  $\text{CuFeO}_2$  high-pressure phase as a result of Hund's rule breakdown at very high density. Such a transition will be accompanied by a significant reduction of the TM ionic radii and therefore a volume decrease or even a structural transition. Finally, at  $P > 75$  GPa a *Mott* transition occurs in  $\text{CuFeO}_2$  resulting in a metallic phase.

(iii) Sluggish structural phase transitions in antiferromagnetic insulators  $\text{FeI}_2$  and  $\text{FeCl}_2$  attributed to the onset of a *Mott* transition (MT). These studies show a precursor intermediate pressure phase formation preceding the MT and allow establishing features of the structural transformation specifically attributed to the MT for different types of the electronic transitions (Mott-Hubbard and Charge-Transfer).

(iv) Volume dependence of the orbital term of the moment in  $\text{FeI}_2$  and  $\text{FeCl}_2$  results in its eventual collapse under pressure. For these compounds significant lattice distortion is observed attributed to the quenching of the orbital term, and this transformation further culminates into a Mott transition.

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**Keywords: high pressure; crystallographic transition; magnetic/electronic transitions**

#### FA5-MS06-O4

**Total X-ray Scattering Studies of Nanocrystalline and Amorphous Organic and Inorganic Compounds.** D. Beckers<sup>a</sup>, M. Gateshki<sup>a</sup>, J. te Nijenhuis<sup>a</sup>. <sup>a</sup>PANalytical B.V., Lelyweg 1, 7602 EA Almelo, The Netherlands.

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Recent interest in nanomaterials has increased the need to analyze structures on a local (nano) scale. However, the atomic structures of nanostructured and amorphous materials are not accessible by conventional methods used to study crystalline materials, because of the short ordering range in these materials. One of the most promising techniques to study nanostructures using X-ray diffraction is total scattering pair distribution function (PDF) analysis. The pair distribution function provides information of finding atoms separated at a certain distance. This function is not direction dependent; it only looks at the absolute value of the distance between the nearest neighbours, the next nearest neighbours and so on. The method can therefore also be used to analyze non-crystalline materials.

We have developed the application of PDF analysis on a standard laboratory system employing an X-ray tube with a silver anode as X-ray source. Previous measurements have shown that meaningful results have been achieved on various samples of different nature –crystalline, nanocrystalline, amorphous solid and liquid.

In this study we compare PDF calculations on different amorphous materials. We show the analysis of some inorganic samples like geopolymers. As an organic

model substance we used lactose. We present results on the monitoring of crystallization processes of freeze- and spray-dried lactose as well as the analysis of lactose of different constitution (alpha-lactose monohydrate / beta-lactose mixtures).

**Keywords: amorphous compounds; nanocrystallites; pair distribution function**

#### FA5-MS06-O5

**TEM Characterization of Axial CdTe/ZnTe Nanowires and Simulation of Growth by Finite Element Method.** Holm Kirmse<sup>a</sup>, Wolfgang Neumann<sup>a</sup>, Paweł Dłużewski<sup>b</sup>, Sławek Kretc, Tomasz Wojtowicz<sup>c</sup>, Detlef Klimm<sup>d</sup>.

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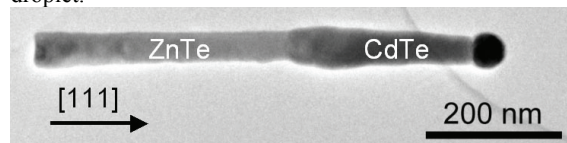
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Nanowires (NWRs) are one-dimensional objects of only some 10 nm diameter and a length up to several micrometres. Semiconductor NWRs exhibit unique physical properties making the NWRs favourable for new applications. Electronic and even photonic functionality can be introduced by a p-n junction in axial heterostructure NWRs. For applications in the infrared range of light a materials combination of CdTe/ZnTe can be chosen.

Such NWRs were fabricated via a vapour-liquid-solid (VLS) growth process generated in a molecular beam epitaxy system. Liquid droplets of a gold-based catalyst promoted the NWR growth. In a first step, ZnTe nanowires were grown. After a growth interruption Cd and Te were provided for the further growth process resulting in NWRs with a CdTe/ZnTe interface.

For the TEM characterization the NWRs were harvested from the substrate and transferred to a holey carbon film. The TEM investigations were performed at a JEOL 2200FS operating at 200 kV.

The NWRs exhibit an unique shape comprising a concentric buckling of the CdTe part close to the interface. The buckling can be attributed to a combination of three effects: first, relaxation of lattice mismatch, second, lateral growth, and third, variation of the size/shape of the catalyst droplet.



TEM bright field image of a harvested CdTe/ZnTe NWR. The CdTe/ZnTe interface is free of misfit dislocations. Hence, a pure elastic relaxation of the lattice mismatch has to be considered. CdTe is compressed and relaxes within a

certain distance from the interface. But, the increase of the NWR diameter by far exceeds the lattice mismatch of 6 %. Lateral growth is observed when the NWR length exceeds the path length of the surface diffusion. A portion of the diffusing atoms is consumed for lateral growth. This effect leads to the well-known tapering of NWRs. The expected formation of a Cd-rich shell in the buckled region is not found. Hence, the buckling is not due to a lateral growth. Conclusively, only a variation of either the size or shape of the catalyst droplet can cause the buckling. By altering growth parameters like temperature or droplet composition the properties of the liquid droplet are modified. This can cause a different diameter or even an ellipsoidal shape of the droplet leading to an enlarged liquid/solid interface area.

**Keywords:** semiconductor; nanowire; axial heterostructure

#### FA5-MS06-O6

**X-ray Absorption Spectroscopy: A Powerful Tool to Probe the Zr Shift Towards the Centrosymmetric Position in PZT ( $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$ ) Under High Pressure and High Temperature.**  
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Ferroelectrics materials with the perovskite structure have drawn considerable attention for many years.  $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$  (PZT) ceramics have been the subject of numerous studies due to their exceptional ferroelectric properties. These solid solutions exhibit their highest electromechanical responses for compositions ( $x \sim 0.48$ ) lying at the so-called morphotropic phase boundary between the rhombohedral or monoclinic and tetragonal phases. PZT adopts an  $\text{ABO}_3$  perovskite-type structure with chemical disorder on the B site (occupied by Zr and Ti). Intrinsic short range dynamical disorder has been experimentally observed [1] and theoretically predicted [2]. The presence of diffuse X-ray/neutron scattering is clearly observed in  $\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$  diffraction patterns which is an evidence of local lattice deformations with respect to the average structure [3]. Simultaneous high pressure at high temperature X-ray absorption and X-ray diffraction experiments were carried out on BM29 at ESRF to follow the changes in short range order around Zr at the ferro- to para-electric phase transition. Measurements on the 300K isotherm indicate a clear change in the EXAFS signal, between 5.3GPa and 6.1GPa, as well as a decrease of the intensity of the prepeak (observed in spite of a short lifetime of the excited state, 3.83eV). Changes in the XANES in the same pressure range can be reproduced by calculations with the FDMNES code [4]. A noticeable decrease in the Debye-Waller factor

(DWF) is observed above 6GPa, in agreement with DWF for the centrosymmetric  $\text{BaZrO}_3$  [5]. All these features indicates that Zr atoms shift toward the centrosymmetric position between 5.3 and 6.1GPa, corresponding to the ferro-paraelectric transition. Moreover, this pressure range corresponds to the value of the Curie pressure  $P_c$  obtained by neutron diffraction and resonant Raman spectroscopy [3]. Similar results are observed for the 450K isotherm. X-ray absorption is thus the technique of choice to probe the ferro-paraelectric transition at the local scale. It has been possible to observe, through the decrease of the DWF, a very small displacement of the Zr ( $\sim 0.06 \text{ \AA}$ ) from an off-center to a centrosymmetric position.

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**Keywords:** X-ray absorption; X-ray diffraction; piezo- and ferroelectrics materials